How GDA helps to turn raw data into results
Or at least lets you decide if you are collecting reasonable data

Tobias Richter
for the Diamond data acquisition & scientific software teams

NOBUGS 2010 Gatlinburg

diamond

Introduction

@ Diamond

- is the data acquisition system used on (almost) all beamlines
- has integrated visualisation and analysis features
- caters for a wide range of disciplines
- written in Java
- has a Jython scripting interface
- is a client/server based system
- GUI client written using the Eclipse RCP framework
- is open source software, see www.opengda.org

diamond

Integrated Data Acquisition and Processing

- give the user control over the data he is collecting
  by displaying in a meaningful way
- do not waste beamtime on bad samples
- user is more likely analyse the data in more detail and publish
- can be used for decision making in automated experiments
- should not interfere with data collection

diamond

Integrated Data Acquisition and Processing

- give the user control over the data he is collecting
  by displaying in a meaningful way
- do not waste beamtime on bad samples
- user is more likely analyse the data in more detail and publish
- can be used for decision making in automated experiments
- should not interfere with data collection
- collection and processing at the same time?

diamond

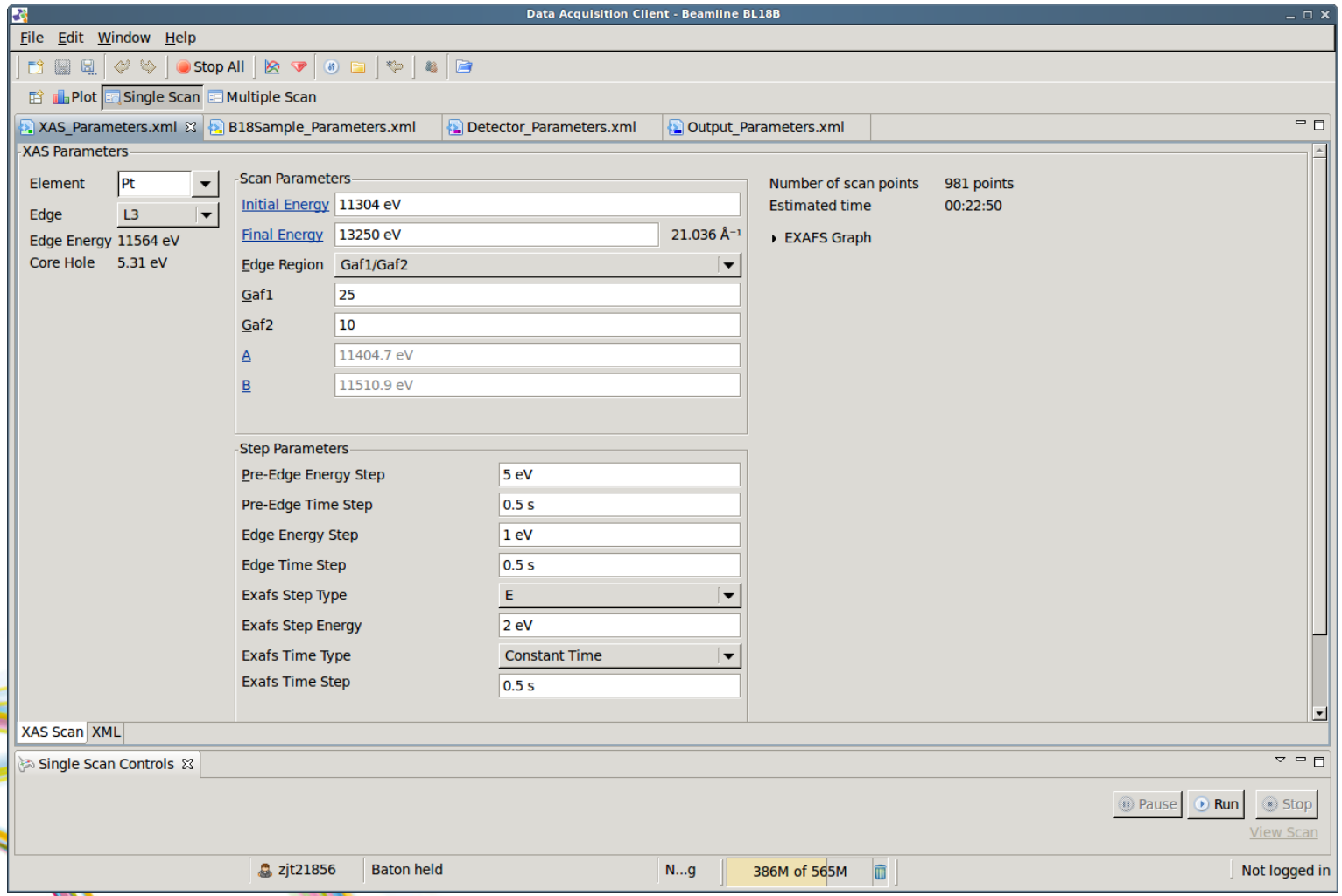
Integrated Data Acquisition and Processing

Exafs Analysis

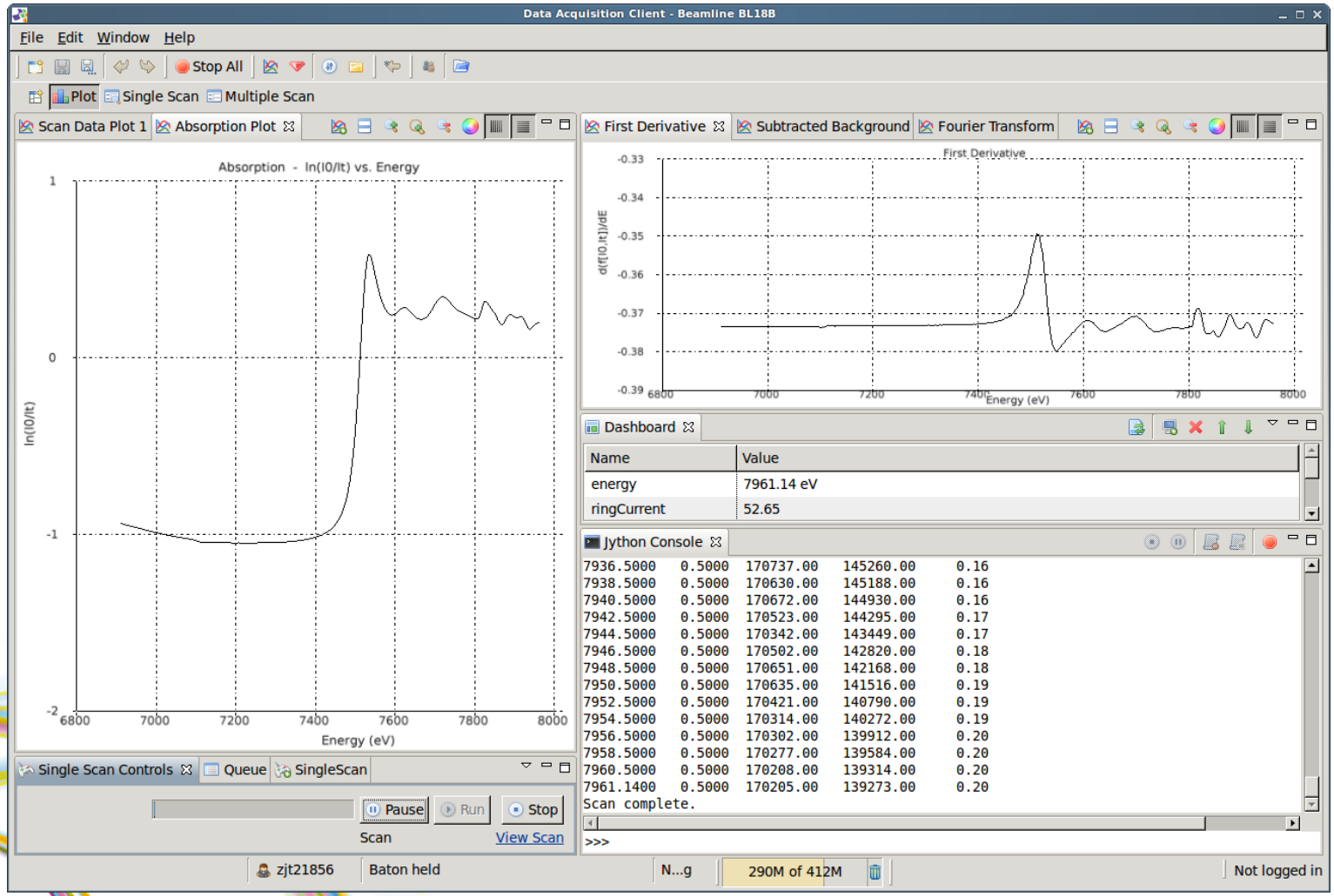
- GUI based
- no processing data is written to the file
- scans with scalar data ($h\nu$ vs. I_0 and I_t) – low data rate
- background subtraction, first derivative and fourier transformation are performed

diamond

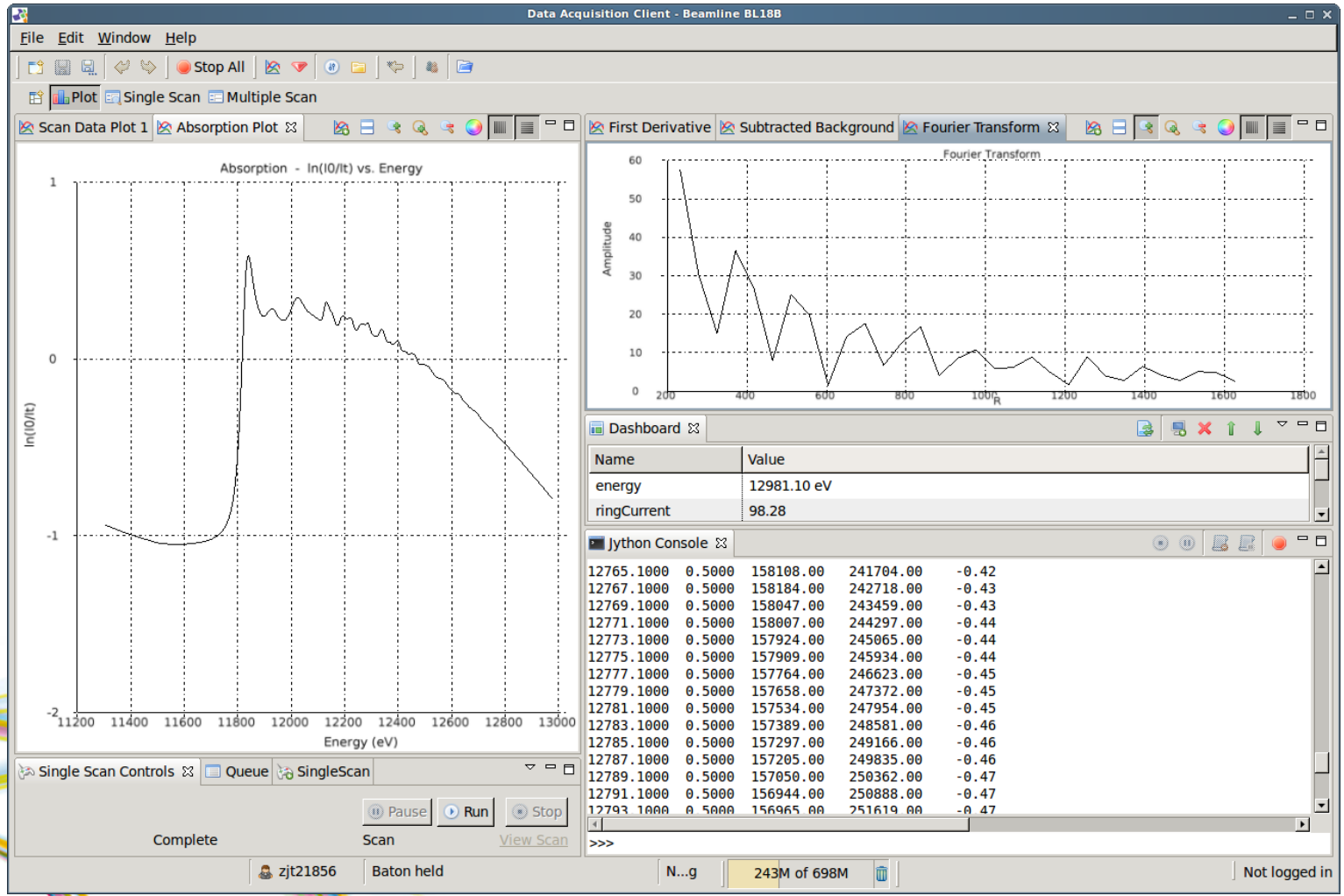
Exafs setup


Data Acquisition Client - Beamline BL18B
File Edit Window Help
Stop All
Plot Single Scan Multiple Scan
XAS_Parameters.xml B18Sample_Parameters.xml Detector_Parameters.xml Output_Parameters.xml
XAS Parameters
Element Pt
Edge L3
Edge Energy 11564 eV
Core Hole 5.31 eV
Scan Parameters
Initial Energy 11304 eV
Final Energy 13250 eV 21.036 Å⁻¹
Edge Region Gaf1/Gaf2
Gaf1 25
Gaf2 10
A 11404.7 eV
B 11510.9 eV
Number of scan points 981 points
Estimated time 00:22:50
EXAFS Graph
Step Parameters
Pre-Edge Energy Step 5 eV
Pre-Edge Time Step 0.5 s
Edge Energy Step 1 eV
Edge Time Step 0.5 s
Exafs Step Type E
Exafs Step Energy 2 eV
Exafs Time Type Constant Time
Exafs Time Step 0.5 s
XAS Scan XML
Single Scan Controls
Pause Run Stop
View Scan
zjt21856 Baton held N...g 386M of 565M Not logged in

Exafs data

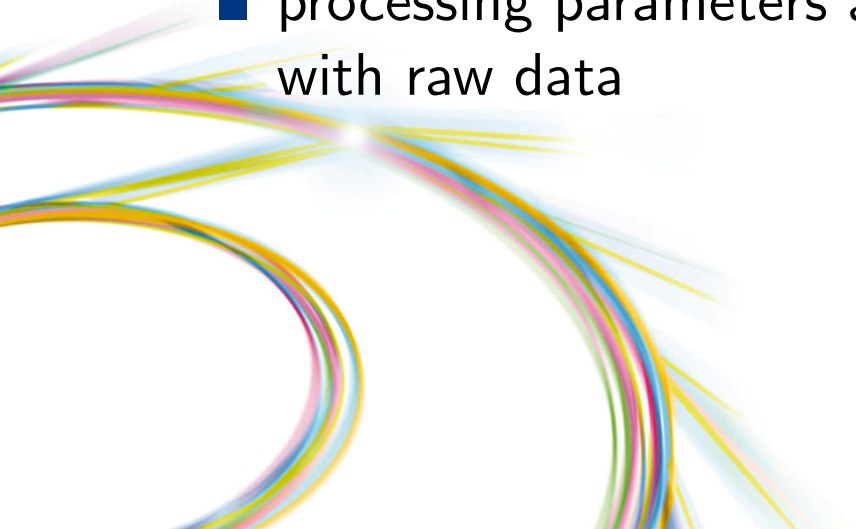

Data Acquisition Client - Beamline BL18B
File Edit Window Help
Stop All
Plot Single Scan Multiple Scan
Scan Data Plot 1 Absorption Plot
Absorption - ln(I0/It) vs. Energy
ln(I0/It)
Energy (eV)
First Derivative Subtracted Background Fourier Transform
First Derivative
d(f[I0,It])/dE
Energy (eV)
Dashboard
Name Value
energy 7961.14 eV
ringCurrent 52.65
Jython Console
7936.5000 0.5000 170737.00 145260.00 0.16
7938.5000 0.5000 170630.00 145188.00 0.16
7940.5000 0.5000 170672.00 144930.00 0.16
7942.5000 0.5000 170523.00 144295.00 0.17
7944.5000 0.5000 170342.00 143449.00 0.17
7946.5000 0.5000 170502.00 142820.00 0.18
7948.5000 0.5000 170651.00 142168.00 0.18
7950.5000 0.5000 170635.00 141516.00 0.19
7952.5000 0.5000 170421.00 140790.00 0.19
7954.5000 0.5000 170314.00 140272.00 0.19
7956.5000 0.5000 170302.00 139912.00 0.20
7958.5000 0.5000 170277.00 139584.00 0.20
7960.5000 0.5000 170208.00 139314.00 0.20
7961.1400 0.5000 170205.00 139273.00 0.20
Scan complete.
>>>
Single Scan Controls Queue SingleScan
Pause Run Stop
Scan View Scan
zjt21856 Baton held N...g 290M of 412M Not logged in

Exafs fourier



Small Angle Scattering

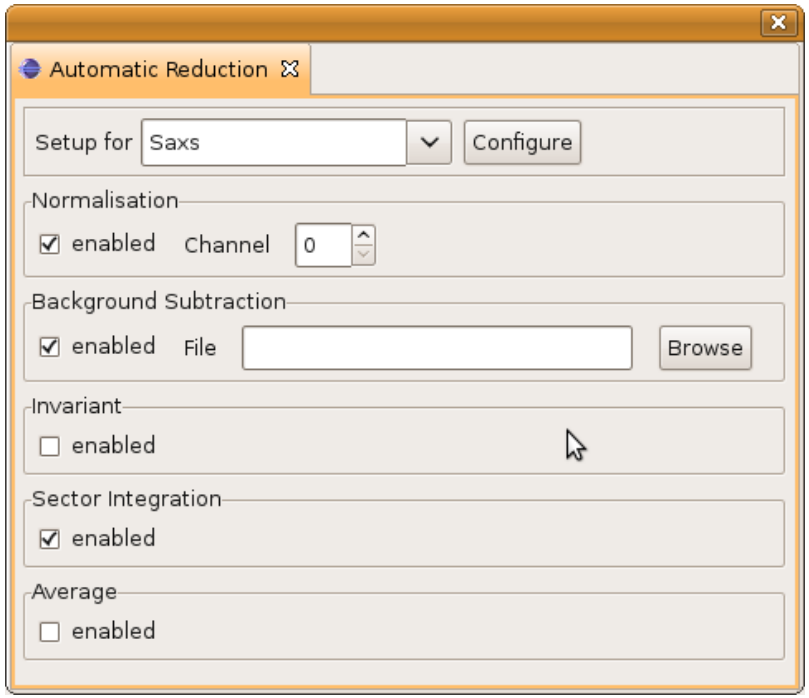
- processing deployed on I22
  which serves physicists, chemists and biologists
- experiments collect from 1MB to 40GB
  and run in 200ms to 4h
- processing runs on server
- processing parameters and results are written to file along with raw data



diamond

Automatic Reduction

- normalise
- detector response
- background subtraction
- average
- invariant
- sector integration



GDA standard tools to visualise and investigate data are used to define reduction parameters (i.e. sector integration)

Data Processing Features

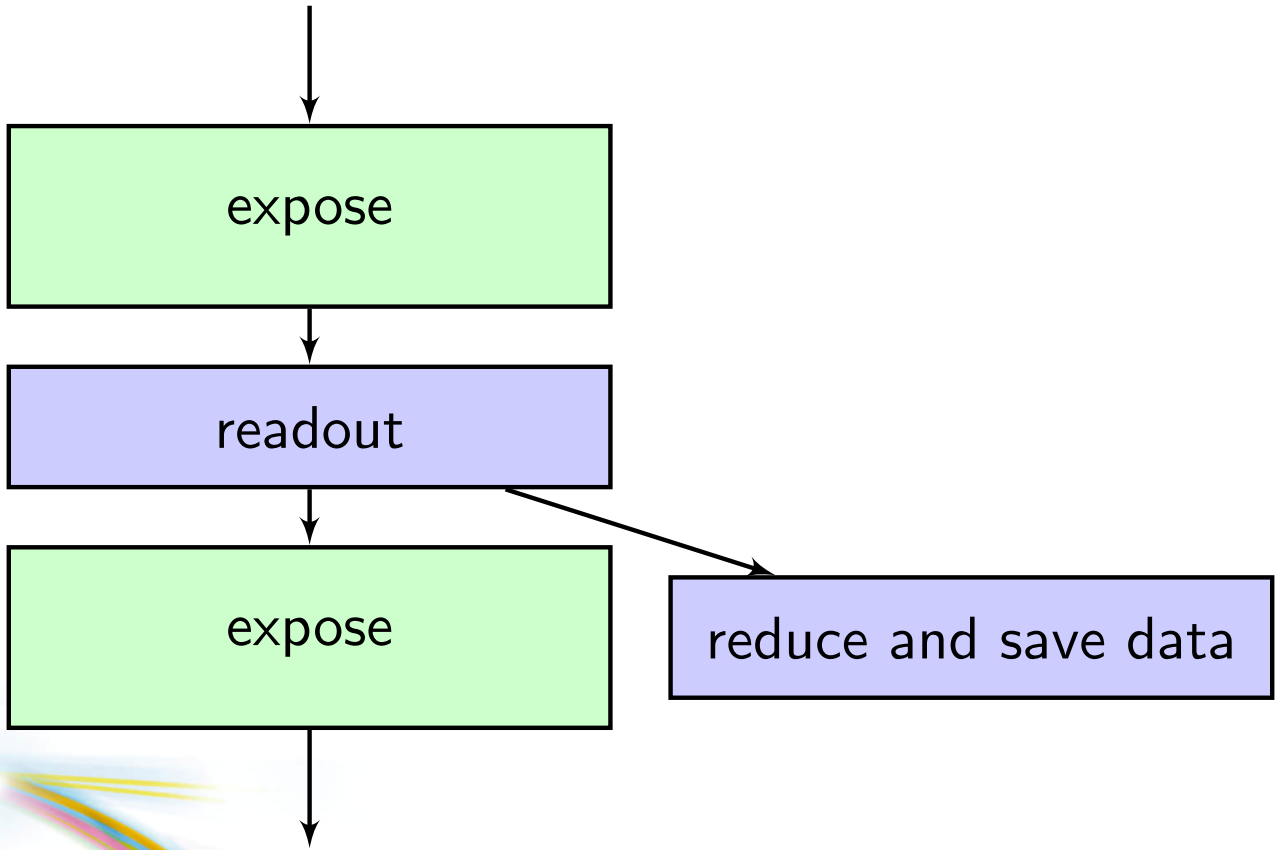
- delivers I vs. q
- reduction results saved to NeXus with raw data
- framework allows any data operation
- extensible (also from scripting) and configurable on the fly
- elements can be combined in a chain or tree
- all data (reduced and raw) for (at least) one frameset needs to fit into memory

diamond

Implementation Details

- detectors present themselves as a detector system with a configureable set of virtual detectors
- each detector (physical or virtual) contributes a partial NeXus tree to the savable data
- each detector receives a handle to the tree structure to read and add data
- when the physical detectors are read, the scan continues
- processing detectors can keep state, if they want to operate across scan point boundaries

Threading



The number of processing threads can be configured at runtime.

Problem

Users need to give up the first few minutes of their beamtime for measuring background, calibrants, etc.

Ongoing Work

- configurable visualisation in domain specific plots (Kratky, Guinier, Porod, Zimm, etc)
- re-evaluation for offline analysis
- simple analysis: peak fitting / finding / following

Outlook

- tuning for performance responsiveness for more exotic cases
- more advanced analysis: domain specific configurable workflow run outside of GDA (using EDNA), results displayed in GDA
- descision making
- deployment on other beamlines (at Diamond and elsewhere)

diamond

Integrated Data Acquisition and Processing

diamond